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THE FORMATION OF AROMATIC AND POLYCYCLIC AROMATIC HYDROCARBONS IN RICH, PREMIXED, LAMINAR FLAMES

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The U.S. Clean Air Act Amendments of 1990 has focused attention on the emission of 189 compounds called air toxic species. Many of these compounds are aromatic hydrocarbons and polycyclic aromatic hydrocarbons (PAH). In the present collaborative research program, PAH formation was investigated in the well controlled, well-characterized environment of a laboratory burner, and the experimental results were used to develop a new chemical kinetic mechanism for PAH formation. Species profiles were measured in a rich, sooting, premixed, atmospheric, laminar flames for methane, ethene and ethane. A GC/MS analytic system was used to obtain concentration measurements of a wide spectrum of aromatics and PAH's. The modeling results show that the key step leading to benzene in these flames is $H_2CCCH\ F \rightarrow C_6H_5$(phenyl) + H. Additionally, new reaction steps involving the recombination of resonantly stabilized radicals have been used to describe the formation of substituted aromatics and PAH's.

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